Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supporting Information

A New Anthraquinone Derivative as Near UV and Visible Light Photoinitiator for Free-Radical, Thiol-ene and Cationic Polymerizations

Yi Zhu,[a, b] Junyi Pi,[a] Yuchao Zhang,[d] Dandan Xu,[a] Yusuf Yagci [b, c] and Ren Liu*[a,b]

[a] *Key Laboratory of Synthetic and Biological Colloids, Ministry of Education, School of Chemical and Material Engineering, Jiangnan University, 214122, Wuxi, Jiangsu (P. R. China)*
E-mail: liuren@jiangnan.edu.cn.

[b] *International Research Center for Photoresponsive Molecules and Materials, Jiangnan University, 214122, Wuxi, Jiangsu (P. R. China).*

[c] *Department of Chemistry, Faculty of Science and Letters, Istanbul Technical University, 34469, Maslak, Istanbul (Turkey).*

[d] *School of Chemistry and Chemical Engineering, Nanjing University, 210023 Nanjing, Jiangsu (P. R. China)*

Table of Contents:

Synthesis of Q2 Q3 Q3-Me Q4

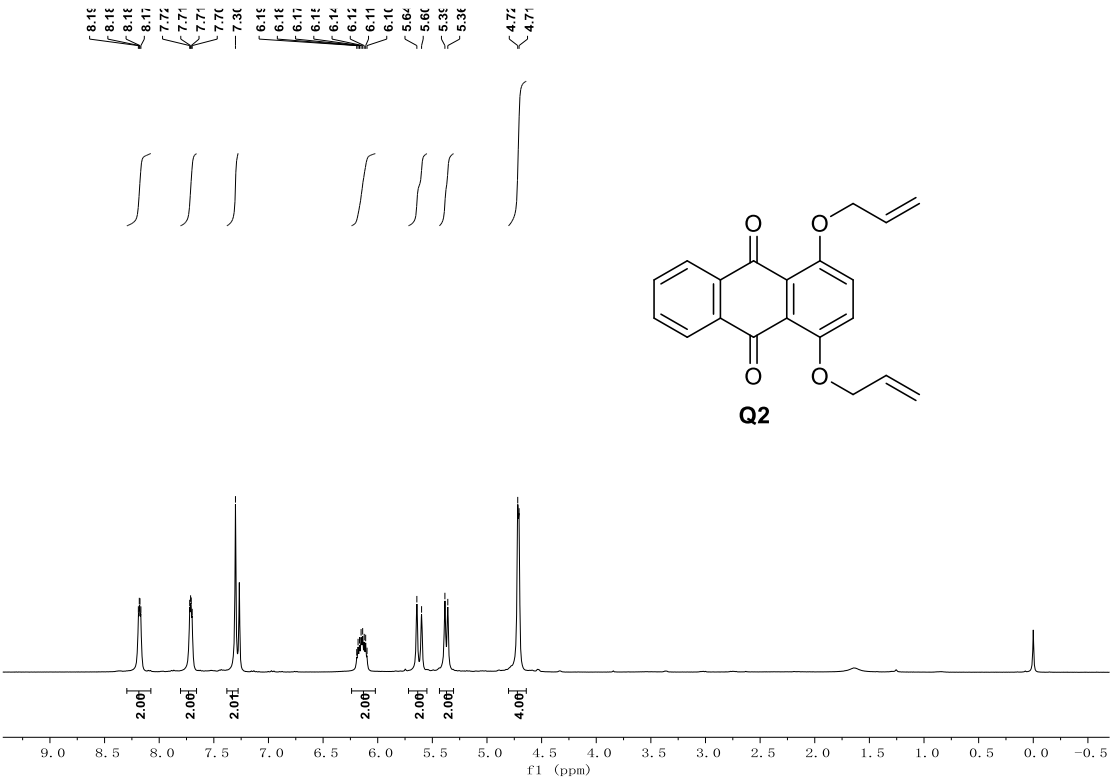
Synthesis of allyl quinizarin (Q2): K_2CO_3 (3.32 g, 24 mmol, 16 equiv) and allyl bromide (12 mL, 92 equiv) and 1,4-dihydroxyanthraquinone (Q1) (720.6 mg, 3.0 mmol, 2 equiv) were dissolved in acetone (150 mL) and stirred at 58 ^oC under reflux for 20 h. The reaction was monitored by TLC. After the starting materials Q1 was completely consumed, H_2O was added (150 mL) into the reaction mixture and the system was extracted with Et_2O (3 × 60 mL). Then, combined the organic phase was washed with H_2O and brine solution. Finally, the organic phase was dried and concentrated under reduced pressure, and the residue was purified by chromatography (PE/ EtOAc = 4/1) to afford product allyl quinizarin (Q2) as a yellow powder (80%). ^{1}H NMR (400 MHz, CD_3Cl) δ 8.18 (dd, J = 5.9, 3.4 Hz, 2H), 7.71 (dd, J = 5.8, 3.4 Hz, 2H), 7.30 (s, 2H), 6.15 (ddt, J = 16.0, 10.3, 5.0 Hz, 2H), 5.62 (d, J = 17.3 Hz, 2H), 5.37 (d, J = 10.6 Hz, 2H), 4.71 (d, J = 4.9 Hz, 4H); ^{13}C NMR (101 MHz, CD_3Cl) δ 183.2, 153.3, 134.2, 133.3, 132.6, 126.5, 123.6, 122.2, 118.1, 70.9.

Synthesis of 2,3-diallyl-1,4-dihydroxyanthracene-9,10-dione (Q3): Under argon protection, sodium disulfite (1.04 g, 6.0 mmol) was dissolved in a mixed solvent of water (200 ml) and DMF (100 ml). Then, the mixture was heated to 90 ℃ and the solution of Q2 (0.88 g, 3.0 mmol) in 100 ml DMF was added to the mixture. Afterwards, the above system was heated to reflux for 3 h, then sodium hydroxide (0.30 g, 7.5 mmol) was added. At the end of the reaction under reflux for 45 min, the reaction solution was cooled to room temperature. The system was extracted with EtOAc (3 × 200 mL). The combined organic phase was washed with brine solution (5 × 200 mL). The dried and concentrated under reduced pressure. Finally, the residue was purified by chromatography (PE/ CH_2Cl_2 = 25/1) to afford the target product Q3 as a red solid (82%). ^{1}H NMR (400 MHz, CD_3Cl) δ 13.59 (s, 2H), 8.35 (dd, *J* = 5.8, 3.3 Hz, 2H), 7.82 (dd, *J* = 5.9, 3.3 Hz, 2H), 5.98 (ddt, *J* = 16.4, 12.0, 5.1 Hz, 2H), 5.38 – 5.04 (m, 4H), 3.59 (dt, *J* = 6.0, 1.7 Hz, 4H); ^{13}C NMR (101 MHz, CD_3Cl) δ 186.6, 157.1, 139.8, 134.2, 133.6, 126.9, 120.0, 116.3, 110.8, 30.5.

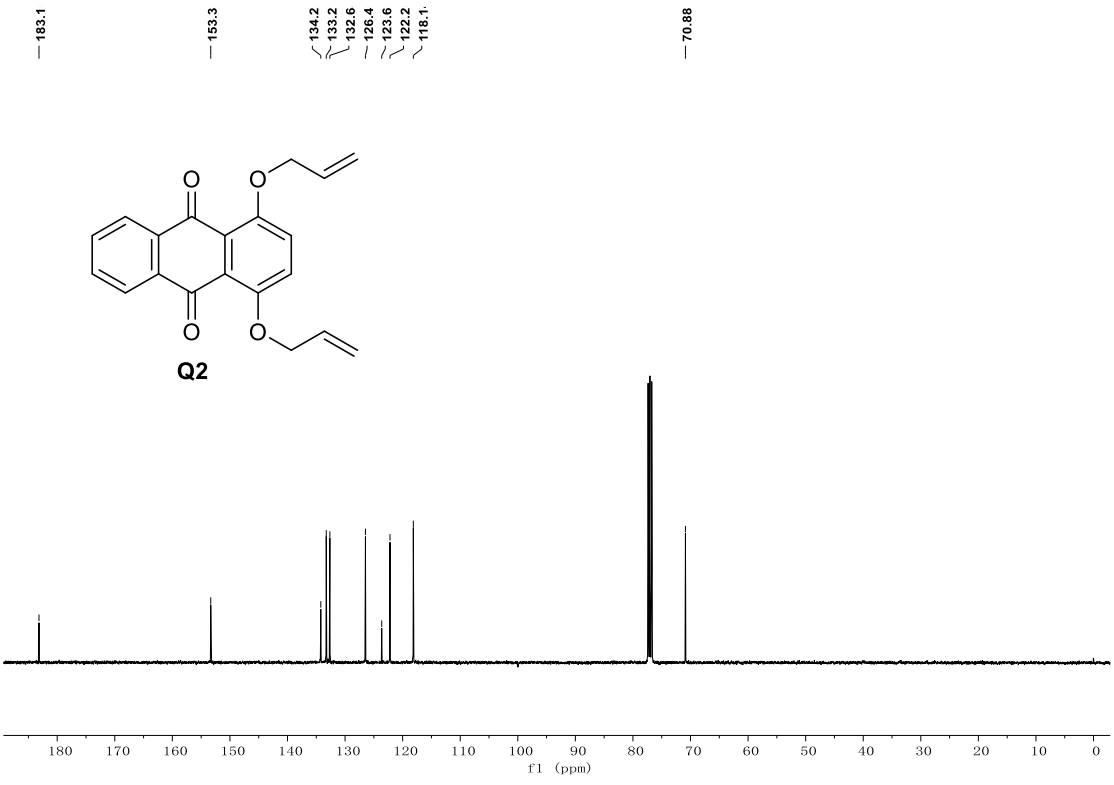
Synthesis of 2,3-diallyl-1,4-dimethoxyanthracene-9,10-dione (Q3-Me): Q3 (204 mg, 0.64 mmol) was dissolved in in dry acetone (100 ml), then methyl iodide (0.4 mL, 6.4 mmol) and potassium carbonate (442 mg, 3.2 mmol) were added. The reaction system was allowed to stir at room temperature for 18 h. The reaction was monitored by TLC until Q3 completely consumed and then filtered through a celite pad. The residue was washed with dichloromethane (3 × 20 mL). Evaporation of the solvent gave the crude product, which was purified by chromatography (PE/ EtOAc = 97/3) to afford the target product Q3-Me as a yellow liquid (95%).^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (dt, J = 6.9, 3.4 Hz, 2H), 7.73 (dd, J = 5.9, 3.3 Hz, 2H), 5.98 (ddt, J = 17.1, 10.2, 5.7 Hz, 2H), 5.07 (dd, J = 10.2, 1.7 Hz, 2H), 4.94 (dq, J = 17.2, 1.8 Hz, 2H), 3.90 (s, 6H), 3.58 (dt, J = 5.7, 1.9 Hz, 4H).

Synthesis of 6,11-dimethoxy-7,10-dihydrotetracene-5,12-dione (Q4): Under argon protection, Q3-Me (245 mg, 0.704 mmol) and Grubbs I (20.6 mg) were dissolved in dry dichloromethane (15 ml). The reaction system was stirred at room temperature for 2 h. The reaction mixture was concentrated under reduced pressure, and the residue was purified by chromatography (PE/ EtOAc = 10/1) to afford the target product Q4 (75%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 – 7.99 (m, 2H), 7.86 - 7.49 (m, 2H), 5.93 (s, 2H), 3.92 (s, 6H), 3.49 (s, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 183.0, 154.9, 138.9, 133.5, 126.5, 124.4, 123.1, 61.4, 24.9.

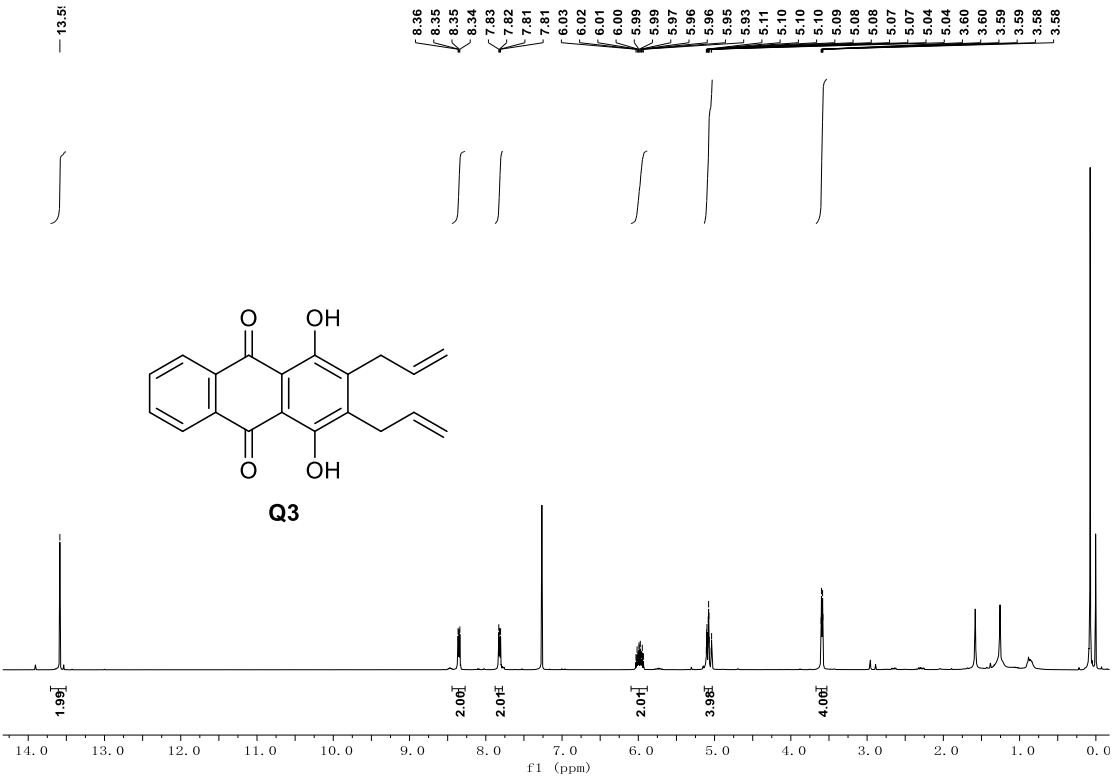
^{1}H NMR and ^{13}C NMR Spectra



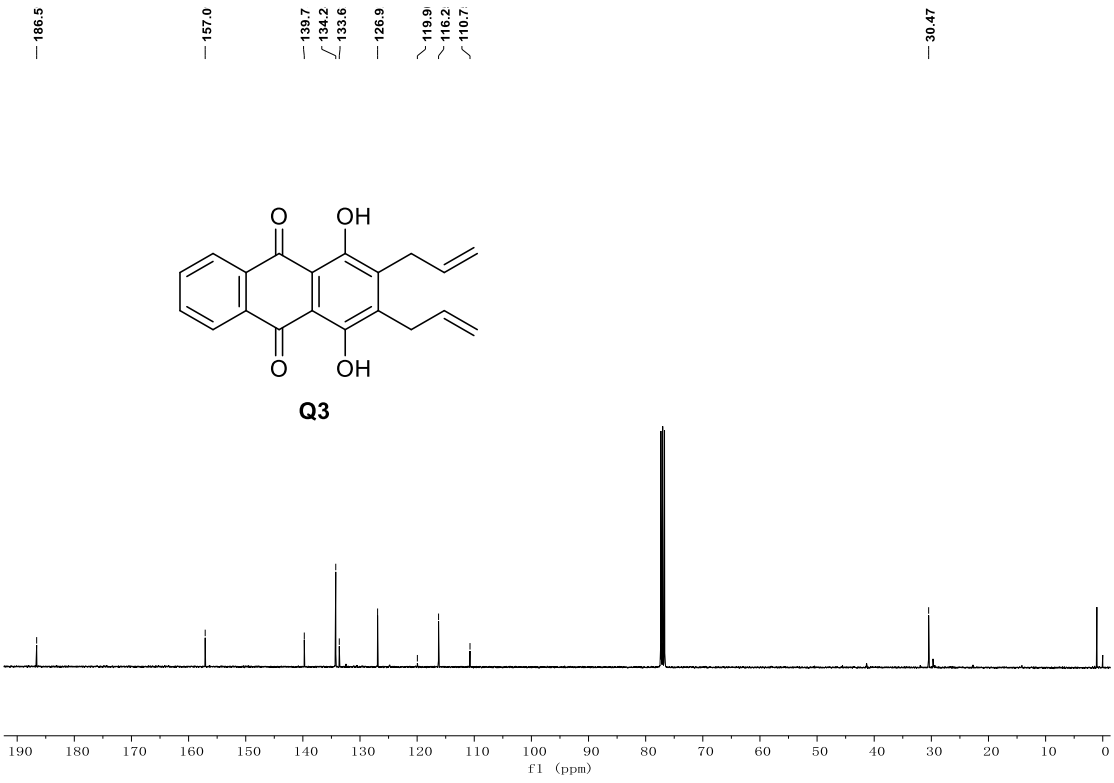
Q2



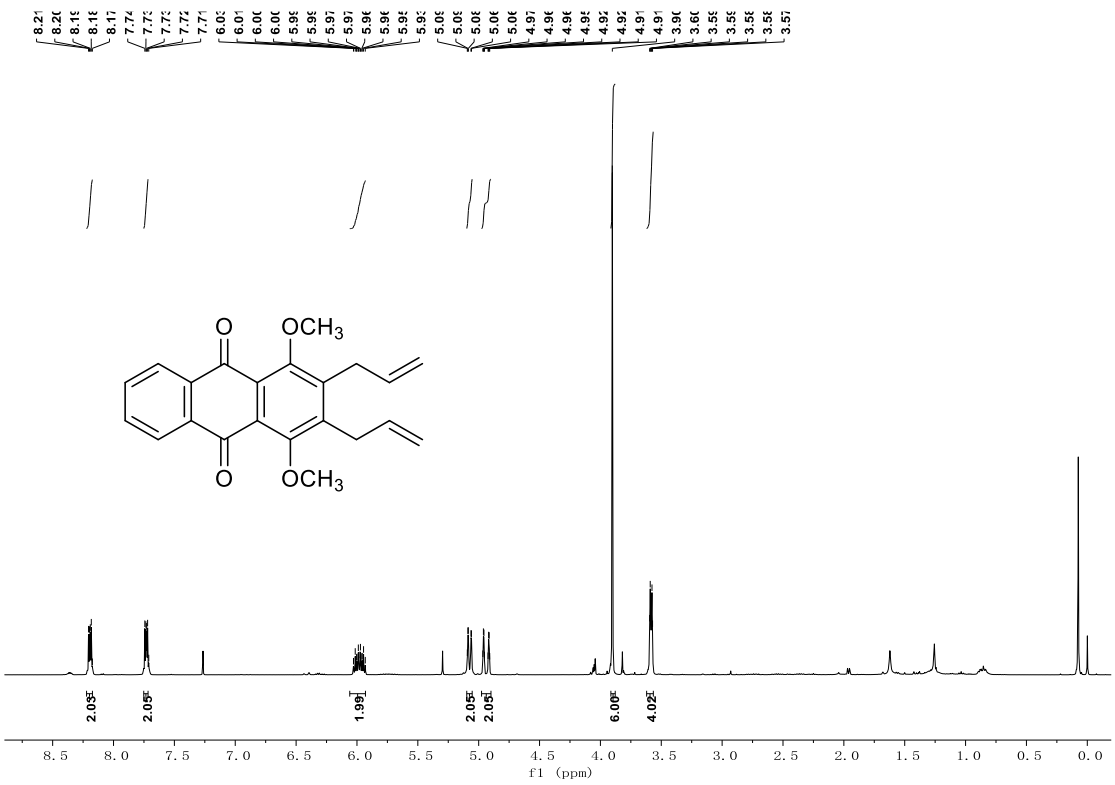
Q2

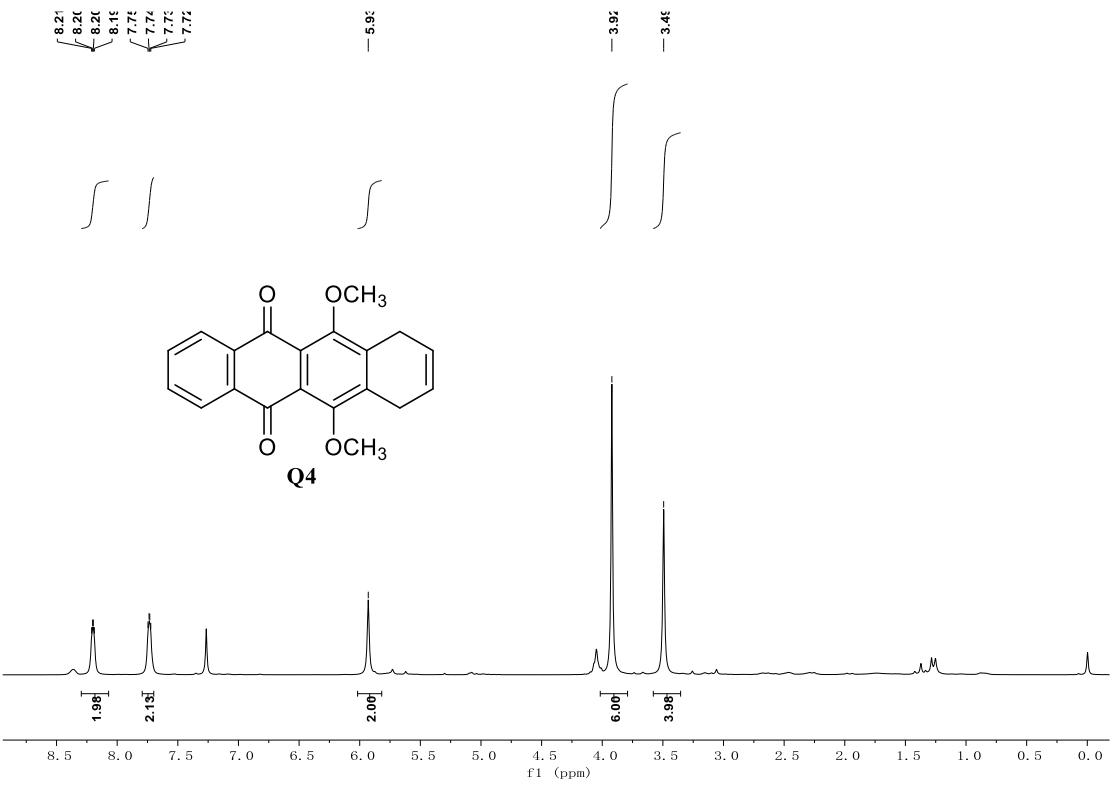

13.58
8.36
8.35
8.35
8.34
7.83
7.82
7.81
7.81
6.03
6.02
6.01
6.00
5.99
5.99
5.97
5.96
5.96
5.95
5.93
5.11
5.10
5.10
5.09
5.08
5.08
5.07
5.07
5.04
5.04
3.60
3.60
3.59
3.59
3.58
3.58
O
OH
O
OH
1.99
2.06
2.01
2.01
3.98
4.06
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

Q3

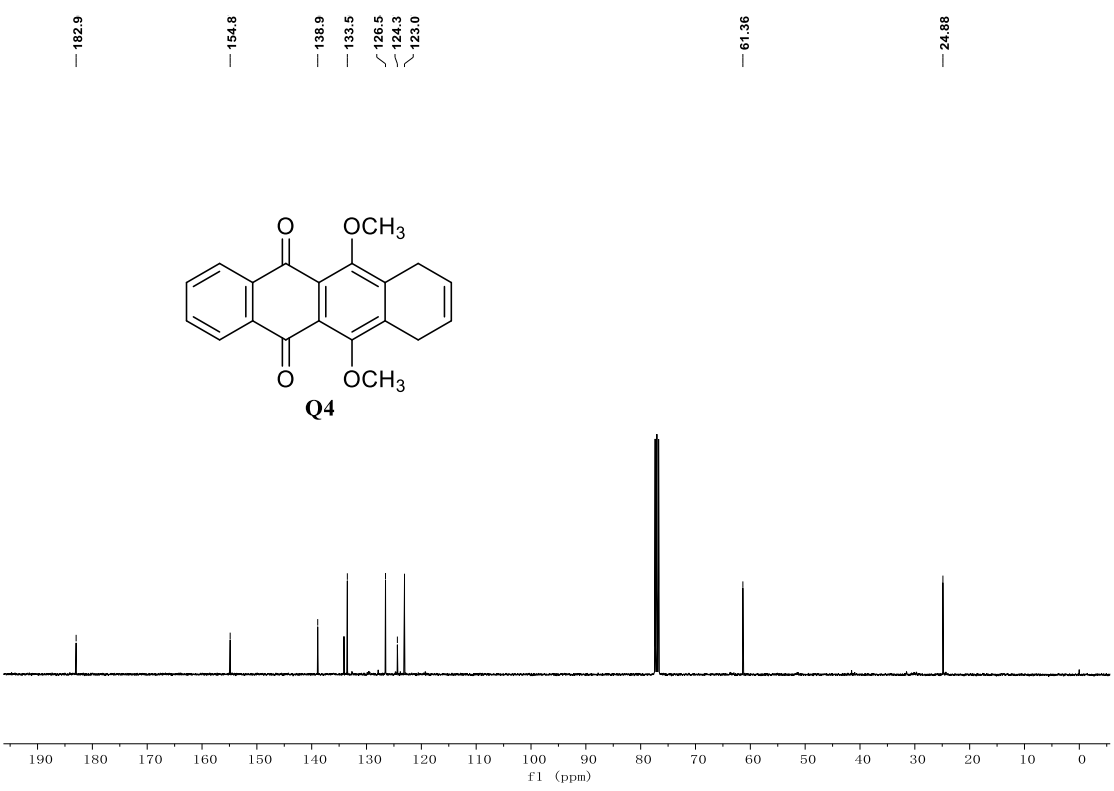

186.5
157.0
139.7
134.2
133.6
126.9
119.9
116.2
110.7
30.47
O
OH
O
OH
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Q3


O
OCH3
O
OCH3
2.05
2.05
1.99
2.05
2.05
6.00
4.02
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


8.21
8.20
8.20
8.19
7.75
7.74
7.72
7.72
5.93
3.92
3.45
O
OCH3
O
OCH3
1.98
2.13
2.00
6.00
3.98
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

Q4


182.9
154.8
138.9
133.5
126.5
124.3
123.0
61.36
24.88
O
OCH3
O
OCH3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

Q4

Hole-electron analysis

Figure S1 Hole-electron analysis on S_1 state of Q2, Q3 and Q4. (A) Structure and atom number for no-hydrogen atoms of Q2, Q3 and Q4; (B) Real space representation of hole and electron distributions of Q2, Q3 and Q4 (isovalue = 0.003 a. u.). Green and blue regions denote the hole and electron distributions, respectively; (C) Real space representation of C_{hold} and C_{ele} functions of Q2, Q3 and Q4 (isovalue = 0.002 a. u.); (D) Heat map of hole and electron contributions of Q2, Q3 and Q4.

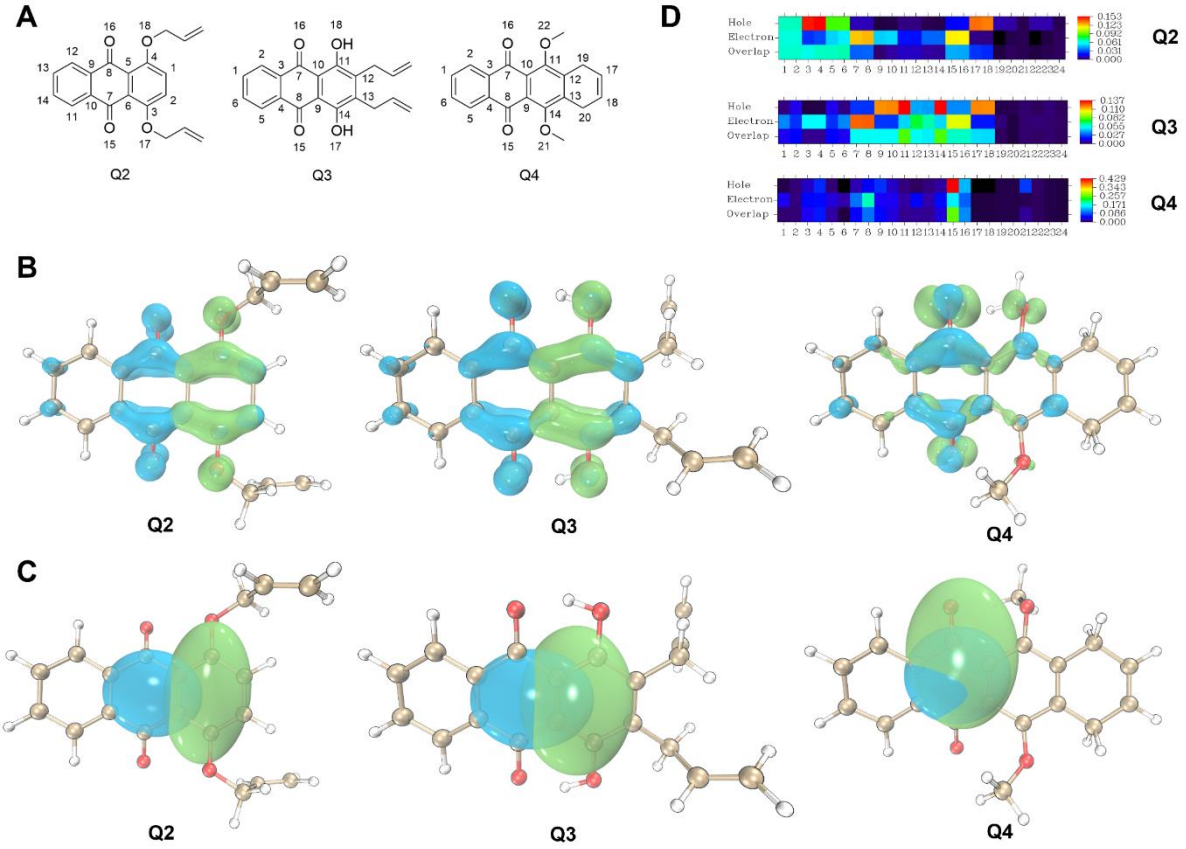


Table S1. Results from hole-electron analysis on S_1 state of Q2, Q3 and Q4.

Compound	Excitation energy (eV)	Sr index (a. u.)	t index (Å)	D index (Å)	Δσ (Å)
Q2	2.800	0.63356	0.441	2.025	0.332
Q3	2.558	0.75079	-0.399	1.390	0.434
Q4	3.006	0.57712	-1.039	0.802	0.210

Computation Results

Describe	Q2 Minimized Geometry at Ground State		
level of opt &freq	PBE0, may-cc-pVTZ, DFT-D3(BJ), IEFPCM(acetonitrile)		
electronic energy		-1071.7840180 a.u.	
Temperature		298.150 K	
Thermal correction to U	874.436 kJ/mol	208.995 kcal/mol	0.333055 a.u.
Thermal correction to H	876.915 kJ/mol	209.588 kcal/mol	0.333999 a.u.
Thermal correction to G	682.963 kJ/mol	163.232 kcal/mol	0.260127 a.u.
Sum of electronic energy and thermal correction to G			
-1071.5238911 a.u.			

```
* xyz  0  1
C        2.15479031     0.88863584    -0.14756555
C        2.27948548    -0.45527081     0.11438031
C        1.16497917    -1.29248506     0.14327228
C        0.91097860     1.46349464    -0.40355242
C       -0.23058509     0.64388418    -0.38070141
C       -0.10368252    -0.74008334    -0.10487712
C       -1.31419954    -1.59544446    -0.06345489
C       -1.57156187     1.22231222    -0.63519021
C       -2.74154747     0.44486868    -0.16703571
C       -2.61770482    -0.91311862     0.10653270
C       -3.73271397    -1.64702448     0.49855010
C       -3.97971312     1.06782864    -0.04796130
C       -5.08005613     0.34125001     0.37034164
C       -4.95635971    -1.01834183     0.64375166
O       -1.27834639    -2.81029759    -0.14954199
O       -1.74341625     2.29112275    -1.19429539
O        1.25300956    -2.59927855     0.44238360
O        0.76333377     2.77373994    -0.66548683
C        2.52758123    -3.17815841     0.70447801
C        3.32297684    -3.40316084    -0.53904222
C        4.61964396    -3.15367315    -0.64786618
C        1.87108294     3.65352070    -0.49298834
C        2.21793827     3.86850182     0.94282792
C        3.45552342     3.86917870     1.41587065
H        3.04693889     1.49496550    -0.14877317
H        3.26585489    -0.85368103     0.29239405
H       -3.62133429    -2.70604782     0.69043025
H       -4.06039413     2.12128220    -0.28135260
H       -6.03994667     0.82984680     0.48166786
```

H	-5.82027911	-1.58539551	0.96718302
H	2.28135156	-4.13774044	1.16303741
H	3.08342121	-2.59221396	1.44208805
H	2.77340610	-3.83552268	-1.37071031
H	5.18471121	-2.71892776	0.17065339
H	5.16476203	-3.38268097	-1.55515533
H	1.52131572	4.58861446	-0.93417607
H	2.73561679	3.31945225	-1.07331681
H	1.37669267	4.06893130	1.60080874
H	4.30739136	3.66622597	0.77445853
H	3.66271042	4.08031271	2.45766847

*

Excited State	1:	Singlet-A	2.7999 eV	442.82 nm	f=0.2879	<S**2>=0.000
Excited State	2:	Singlet-A	2.9768 eV	416.50 nm	f=0.0050	<S**2>=0.000
Excited State	3:	Singlet-A	3.2938 eV	376.41 nm	f=0.0005	<S**2>=0.000
Excited State	4:	Singlet-A	3.8139 eV	325.09 nm	f=0.0011	<S**2>=0.000
Excited State	5:	Singlet-A	4.0301 eV	307.65 nm	f=0.0973	<S**2>=0.000
Excited State	6:	Singlet-A	4.0903 eV	303.12 nm	f=0.0232	<S**2>=0.000
Excited State	7:	Singlet-A	4.4206 eV	280.47 nm	f=0.1977	<S**2>=0.000
Excited State	8:	Singlet-A	4.4680 eV	277.50 nm	f=0.0096	<S**2>=0.000
Excited State	9:	Singlet-A	4.5962 eV	269.75 nm	f=0.0003	<S**2>=0.000
Excited State	10:	Singlet-A	4.6597 eV	266.08 nm	f=0.2246	<S**2>=0.000
Excited State	11:	Singlet-A	4.7850 eV	259.11 nm	f=0.0096	<S**2>=0.000
Excited State	12:	Singlet-A	4.8970 eV	253.18 nm	f=0.1360	<S**2>=0.000
Excited State	13:	Singlet-A	5.1195 eV	242.18 nm	f=0.7135	<S**2>=0.000
Excited State	14:	Singlet-A	5.1729 eV	239.68 nm	f=0.0074	<S**2>=0.000
Excited State	15:	Singlet-A	5.1971 eV	238.56 nm	f=0.0184	<S**2>=0.000
Excited State	16:	Singlet-A	5.2504 eV	236.14 nm	f=0.0229	<S**2>=0.000
Excited State	17:	Singlet-A	5.3903 eV	230.01 nm	f=0.0239	<S**2>=0.000
Excited State	18:	Singlet-A	5.4198 eV	228.76 nm	f=0.0899	<S**2>=0.000
Excited State	19:	Singlet-A	5.5628 eV	222.88 nm	f=0.2210	<S**2>=0.000
Excited State	20:	Singlet-A	5.5769 eV	222.32 nm	f=0.0449	<S**2>=0.000
Excited State	21:	Singlet-A	5.6840 eV	218.13 nm	f=0.0024	<S**2>=0.000
Excited State	22:	Singlet-A	5.7875 eV	214.23 nm	f=0.0066	<S**2>=0.000
Excited State	23:	Singlet-A	5.8150 eV	213.21 nm	f=0.0178	<S**2>=0.000
Excited State	24:	Singlet-A	5.8467 eV	212.06 nm	f=0.0240	<S**2>=0.000
Excited State	25:	Singlet-A	5.8831 eV	210.74 nm	f=0.0702	<S**2>=0.000

Describe	Q2 Minimized Geometry at S_1 State		
level of opt &freq	PBE0, may-cc-pVTZ, DFT-D3(BJ), IEFPCM(acetonitrile)		
electronic energy		-1071.69099444 a.u.	
Temperature		298.150 K	
Thermal correction to U	870.123 kJ/mol	207.964 kcal/mol	0.331412 a.u.
Thermal correction to H	872.602 kJ/mol	208.557 kcal/mol	0.332357 a.u.
Thermal correction to G	678.693 kJ/mol	162.212 kcal/mol	0.258501 a.u.
Sum of electronic energy and thermal correction to G			
-1,071.702493 a.u.			

```
* xyz  0  1
C         2.25629658      0.70866474     -0.24771533
C         2.27205701     -0.64968854     -0.00238439
C         1.07755426     -1.33702901      0.20164118
C         1.04595862      1.39785123     -0.29634414
C        -0.20850300      0.68373723     -0.25645331
C        -0.19197084     -0.68256565     -0.01096192
C        -1.45062150     -1.47056138     -0.00324635
C        -1.48713138      1.39616375     -0.50693287
C        -2.69124357      0.68574397     -0.12445724
C        -2.67403111     -0.70338127      0.11802249
C        -3.88042526     -1.36471902      0.39742095
C        -3.91387094      1.37400490     -0.07861086
C        -5.08026644      0.71542275      0.22957926
C        -5.06336948     -0.66863205      0.46970634
O        -1.45710496     -2.70471173     -0.11035624
O        -1.52623260      2.52210073     -1.02141212
O         1.02565110     -2.57594616      0.64947550
O         0.96839188      2.71290815     -0.33755275
C         2.21997591     -3.36124270      0.78253505
C         2.76028345     -3.78460746     -0.54141373
C         4.04261015     -3.71326859     -0.86519157
C         2.14996305      3.51869201     -0.45360252
C         2.83698214      3.68729250      0.86015880
C         4.14909775      3.59667716      1.01612304
H         3.19174704      1.24335958     -0.29110141
H         3.21940298     -1.15018708      0.12000364
H        -3.85237174     -2.43437632      0.56092310
H        -3.91169899      2.43643354     -0.28607962
H        -6.01378066      1.26190607      0.28459544
H        -5.98392945     -1.18661687      0.70927808
H         1.88283359     -4.22619370      1.35364436
```

H	2.96040220	-2.82327662	1.37814772
H	2.03550215	-4.20694351	-1.23090787
H	4.77832590	-3.29380787	-0.18666857
H	4.40311465	-4.08109406	-1.81765019
H	1.76295571	4.47550656	-0.80578207
H	2.81288431	3.11247999	-1.21935752
H	2.19366373	3.94076180	1.69736147
H	4.80475860	3.34571510	0.18871364
H	4.61447424	3.78019797	1.97640752

*

Describe	Q3 Minimized Geometry at Ground State		
level of opt &freq	PBE0, may-cc-pVTZ, DFT-D3(BJ), IEFPCM(acetonitrile)		
electronic energy		-1071.8640490 a.u.	
Temperature		298.150 K	
Thermal correction to U	875.504 kJ/mol	209.250 kcal/mol	0.333462 a.u.
Thermal correction to H	877.983 kJ/mol	209.843 kcal/mol	0.334406 a.u.
Thermal correction to G	693.269 kJ/mol	165.695 kcal/mol	0.264052 a.u.
Sum of electronic energy and thermal correction to G			
-1071.5999969 a.u.			

* xyz 0 1

C	-5.32768410	0.76886396	0.21258411
C	-4.10951194	1.41097103	0.34756808
C	-2.92414320	0.70289658	0.17929883
C	-2.96864334	-0.66282443	-0.12705589
C	-4.19775423	-1.30018815	-0.26084826
C	-5.37185341	-0.58789994	-0.09197041
C	-1.63588946	1.40042860	0.32561383
C	-1.72815021	-1.43415638	-0.30876736
C	-0.46502310	-0.74286183	-0.16661276
C	-0.41954065	0.63822731	0.14291315
C	0.81616977	1.27218093	0.27752017
C	2.02352186	0.54670006	0.11139945
C	1.97844051	-0.79509399	-0.20657932
C	0.72666078	-1.44754819	-0.33517501
H	-6.24772410	1.32404652	0.34442307
H	-4.05823420	2.46531457	0.58413658
H	-4.21520604	-2.35557190	-0.49771372
H	-6.32628903	-1.08798834	-0.19711980
O	-1.77697167	-2.64657229	-0.57607096
O	-1.60705194	2.61216518	0.59846521
O	0.89975111	2.56592218	0.57066221
H	-0.04432607	2.88076790	0.64990037
O	0.72786972	-2.74710902	-0.61935837
H	-0.23496273	-3.00754629	-0.66910672
C	3.22351112	-1.61910020	-0.39130291
H	3.00980816	-2.40232524	-1.12202011
H	4.03442364	-1.01286996	-0.79264556
C	3.32115646	1.28942424	0.26616571
H	3.19325074	2.09504753	0.98847984
H	4.07818503	0.61013651	0.66285107
C	3.78332444	1.86206614	-1.04192176

H	3.95705212	1.14707851	-1.84250224
C	3.97455856	3.15378122	-1.26987227
H	3.79910420	3.89557503	-0.49792951
H	4.31290948	3.51134501	-2.23496967
C	3.65024562	-2.25385220	0.89893050
H	2.90348482	-2.86992732	1.39267989
C	4.84636982	-2.10066644	1.45051986
H	5.61269341	-1.49079308	0.98279377
H	5.10246114	-2.58562778	2.38471177

*

Excited State	1:	Singlet-A	2.5585 eV	484.60 nm	f=0.4062	<S**2>=0.000
Excited State	2:	Singlet-A	3.1883 eV	388.87 nm	f=0.0017	<S**2>=0.000
Excited State	3:	Singlet-A	3.4094 eV	363.65 nm	f=0.0281	<S**2>=0.000
Excited State	4:	Singlet-A	3.6740 eV	337.46 nm	f=0.0006	<S**2>=0.000
Excited State	5:	Singlet-A	3.7703 eV	328.84 nm	f=0.0169	<S**2>=0.000
Excited State	6:	Singlet-A	3.8697 eV	320.40 nm	f=0.0997	<S**2>=0.000
Excited State	7:	Singlet-A	3.9091 eV	317.17 nm	f=0.0028	<S**2>=0.000
Excited State	8:	Singlet-A	3.9309 eV	315.41 nm	f=0.0068	<S**2>=0.000
Excited State	9:	Singlet-A	4.2236 eV	293.55 nm	f=0.3724	<S**2>=0.000
Excited State	10:	Singlet-A	4.6724 eV	265.35 nm	f=0.0097	<S**2>=0.000
Excited State	11:	Singlet-A	4.8512 eV	255.58 nm	f=0.3841	<S**2>=0.000
Excited State	12:	Singlet-A	4.9364 eV	251.16 nm	f=0.7349	<S**2>=0.000
Excited State	13:	Singlet-A	5.1402 eV	241.21 nm	f=0.0200	<S**2>=0.000
Excited State	14:	Singlet-A	5.2818 eV	234.74 nm	f=0.0660	<S**2>=0.000
Excited State	15:	Singlet-A	5.3458 eV	231.93 nm	f=0.0174	<S**2>=0.000
Excited State	16:	Singlet-A	5.3775 eV	230.56 nm	f=0.0035	<S**2>=0.000
Excited State	17:	Singlet-A	5.4611 eV	227.03 nm	f=0.0078	<S**2>=0.000
Excited State	18:	Singlet-A	5.4824 eV	226.15 nm	f=0.0182	<S**2>=0.000
Excited State	19:	Singlet-A	5.4969 eV	225.55 nm	f=0.0373	<S**2>=0.000
Excited State	20:	Singlet-A	5.5685 eV	222.65 nm	f=0.0088	<S**2>=0.000
Excited State	21:	Singlet-A	5.6743 eV	218.50 nm	f=0.0850	<S**2>=0.000
Excited State	22:	Singlet-A	5.7544 eV	215.46 nm	f=0.0020	<S**2>=0.000
Excited State	23:	Singlet-A	5.8383 eV	212.36 nm	f=0.0286	<S**2>=0.000
Excited State	24:	Singlet-A	5.8420 eV	212.23 nm	f=0.0017	<S**2>=0.000
Excited State	25:	Singlet-A	5.9059 eV	209.93 nm	f=0.3038	<S**2>=0.000

Describe	Q3 Minimized Geometry at S_1 State		
level of opt &freq	PBE0, may-cc-pVTZ, DFT-D3(BJ), IEFPCM(acetonitrile)		
electronic energy		-1071.77755068 a.u.	
Temperature		298.150 K	
Thermal correction to U	867.163 kJ/mol	207.257 kcal/mol	0.330285 a.u.
Thermal correction to H	869.642 kJ/mol	207.850 kcal/mol	0.331229 a.u.
Thermal correction to G	683.256 kJ/mol	163.302 kcal/mol	0.260239 a.u.
Sum of electronic energy and thermal correction to G			
-1,071.5173117 a.u.			

* xyz 0 1

C	-5.33357940	0.77746178	0.21731029
C	-4.12035357	1.41462701	0.35374541
C	-2.92031565	0.71057510	0.18469526
C	-2.96769560	-0.67115151	-0.12960191
C	-4.21332938	-1.29963415	-0.26353783
C	-5.38037100	-0.58875348	-0.09314148
C	-1.66258668	1.39314929	0.33233624
C	-1.75953261	-1.42992772	-0.31177986
C	-0.48270317	-0.72982605	-0.16342007
C	-0.43595540	0.61635254	0.14402062
C	0.84037504	1.25633595	0.27946651
C	2.04357109	0.54236155	0.11475389
C	1.99588380	-0.81133248	-0.20846754
C	0.74639134	-1.44778263	-0.33428936
H	-6.25343255	1.33282409	0.35011929
H	-4.07175491	2.46874826	0.59347017
H	-4.23684187	-2.35455752	-0.50368121
H	-6.33631615	-1.08586115	-0.19926252
O	-1.76649581	-2.65765000	-0.59037632
O	-1.58611817	2.61762041	0.61345187
O	0.87703585	2.53605036	0.56603750
H	-0.10877902	2.82124476	0.64128898
O	0.69580395	-2.73066490	-0.60865441
H	-0.30871685	-2.95366305	-0.65531962
C	3.23579229	-1.64092984	-0.38744833
H	3.01376307	-2.44827711	-1.08901650
H	4.03870872	-1.04566765	-0.82197613
C	3.33756791	1.28854288	0.25937475
H	3.21478432	2.09706270	0.98010056
H	4.09990053	0.61238082	0.65184993
C	3.78460081	1.85830973	-1.05618886

H	3.96131040	1.13998563	-1.85294835
C	3.95402394	3.15153699	-1.29389063
H	3.77446076	3.89579430	-0.52520972
H	4.27871582	3.50790070	-2.26413892
C	3.68738061	-2.23175834	0.91641810
H	2.95444702	-2.84269996	1.43663294
C	4.88714831	-2.04609672	1.45009464
H	5.64033149	-1.44009775	0.95669940
H	5.15973651	-2.50032328	2.39502338

*

Describe	Q4 Minimized Geometry at Ground State		
level of opt &freq	PBE0, may-cc-pVTZ, DFT-D3(BJ), IEFPCM(acetonitrile)		
electronic energy		-1071.8271220 a.u.	
Temperature		298.150 K	
Thermal correction to U	878.578 kJ/mol	209.985 kcal/mol	0.334633 a.u.
Thermal correction to H	881.057 kJ/mol	210.578 kcal/mol	0.335577 a.u.
Thermal correction to G	697.212 kJ/mol	166.638 kcal/mol	0.265554 a.u.
Sum of electronic energy and thermal correction to G			
-1071.5615682 a.u.			

* xyz 0 1

C	5.04487691	-0.60450835	-0.10926135
C	3.87774128	-1.26076887	0.23904936
C	2.66292110	-0.58501932	0.19486072
C	2.62166976	0.75640555	-0.17543491
C	3.80121821	1.41600530	-0.50513155
C	5.00588922	0.73584070	-0.48217021
C	1.41939716	-1.29629351	0.55047876
C	1.34467773	1.51205253	-0.16659525
C	0.08866294	0.74121885	-0.00153799
C	0.14242649	-0.66966661	0.15661048
C	-1.03629833	-1.41360664	0.07892490
C	-2.28575917	-0.77593978	-0.01915150
C	-2.34519061	0.60411003	-0.07839135
C	-1.16022871	1.35885305	-0.07859759
H	5.98925684	-1.13386828	-0.09047815
H	3.88785900	-2.30073755	0.53766060
H	3.75536667	2.46259446	-0.77499635
H	5.92083740	1.24905056	-0.75037821
O	1.36720607	2.71988071	-0.33111594
O	1.46521774	-2.33963604	1.18211120
C	-4.78540100	-0.86836153	-0.18021561
C	-4.84537510	0.45459182	-0.23202232
H	-5.69915287	-1.45194797	-0.21679789
H	-5.80800733	0.94857481	-0.31074913
C	-3.51288609	-1.63342197	-0.07254149
H	-3.42009525	-2.33376830	-0.91064516
H	-3.53816603	-2.28254672	0.81031627
C	-3.64793355	1.33852514	-0.19167007
H	-3.73831414	2.04696750	0.63966467
H	-3.62119893	1.97727513	-1.08135383
O	-1.31545969	2.70125212	-0.21373593

O	-1.10057052	-2.75833273	0.08505888
C	-1.15242878	3.45334154	0.98278570
H	-0.14150276	3.35107647	1.37716298
H	-1.33389496	4.49353266	0.72053828
H	-1.87956315	3.13603550	1.73547919
C	-0.19818901	-3.52499870	-0.70082411
H	0.55656851	-3.98961484	-0.06969946
H	-0.79344117	-4.28841664	-1.20074962
H	0.29355667	-2.89967485	-1.44850750

*

Excited State	1:	Singlet-A	3.0058 eV	412.49 nm	f=0.0128	<S**2>=0.000
Excited State	2:	Singlet-A	3.0913 eV	401.07 nm	f=0.2433	<S**2>=0.000
Excited State	3:	Singlet-A	3.3606 eV	368.94 nm	f=0.0185	<S**2>=0.000
Excited State	4:	Singlet-A	3.4464 eV	359.75 nm	f=0.0200	<S**2>=0.000
Excited State	5:	Singlet-A	3.9164 eV	316.58 nm	f=0.0134	<S**2>=0.000
Excited State	6:	Singlet-A	4.0387 eV	306.99 nm	f=0.1004	<S**2>=0.000
Excited State	7:	Singlet-A	4.2593 eV	291.09 nm	f=0.0334	<S**2>=0.000
Excited State	8:	Singlet-A	4.3759 eV	283.33 nm	f=0.1084	<S**2>=0.000
Excited State	9:	Singlet-A	4.4914 eV	276.05 nm	f=0.2302	<S**2>=0.000
Excited State	10:	Singlet-A	4.5149 eV	274.61 nm	f=0.2952	<S**2>=0.000
Excited State	11:	Singlet-A	4.5348 eV	273.40 nm	f=0.0844	<S**2>=0.000
Excited State	12:	Singlet-A	4.8962 eV	253.22 nm	f=0.0102	<S**2>=0.000
Excited State	13:	Singlet-A	5.0405 eV	245.97 nm	f=0.1909	<S**2>=0.000
Excited State	14:	Singlet-A	5.0807 eV	244.03 nm	f=0.0015	<S**2>=0.000
Excited State	15:	Singlet-A	5.1187 eV	242.22 nm	f=0.5711	<S**2>=0.000
Excited State	16:	Singlet-A	5.2755 eV	235.02 nm	f=0.0241	<S**2>=0.000
Excited State	17:	Singlet-A	5.4344 eV	228.15 nm	f=0.0842	<S**2>=0.000
Excited State	18:	Singlet-A	5.4440 eV	227.75 nm	f=0.0166	<S**2>=0.000
Excited State	19:	Singlet-A	5.4912 eV	225.79 nm	f=0.0057	<S**2>=0.000
Excited State	20:	Singlet-A	5.6182 eV	220.68 nm	f=0.1635	<S**2>=0.000
Excited State	21:	Singlet-A	5.6543 eV	219.27 nm	f=0.0904	<S**2>=0.000
Excited State	22:	Singlet-A	5.8431 eV	212.19 nm	f=0.0026	<S**2>=0.000
Excited State	23:	Singlet-A	5.8491 eV	211.97 nm	f=0.0002	<S**2>=0.000
Excited State	24:	Singlet-A	5.8768 eV	210.97 nm	f=0.0097	<S**2>=0.000
Excited State	25:	Singlet-A	5.9000 eV	210.14 nm	f=0.0801	<S**2>=0.000

serial number	Q4 Minimized Geometry at S_1 State		
level of opt &freq	PBE0, may-cc-pVTZ, DFT-D3(BJ), IEFPCM(acetonitrile)		
electronic energy		-1071.7294832 a.u.	
Temperature		298.150 K	
Thermal correction to U	873.403 kJ/mol	208.748 kcal/mol	0.332662 a.u.
Thermal correction to H	875.882 kJ/mol	209.341 kcal/mol	0.333606 a.u.
Thermal correction to G	694.097 kJ/mol	165.893 kcal/mol	0.264368 a.u.
Sum of electronic energy and thermal correction to G			
-1071.4651152 a.u.			

```
* xyz  0  1
C      -5.07477236     0.62380305     0.05581800
C      -3.89928428     1.32575610     0.20743201
C      -2.65804619     0.68955405     0.10902201
C      -2.63317419    -0.69487505    -0.14804001
C      -3.83711728    -1.40581810    -0.30253802
C      -5.04150637    -0.75275005    -0.20078801
C      -1.44055911     1.49432111     0.27121102
C      -1.37268510    -1.37092810    -0.24265202
C      -0.17399301    -0.61675005    -0.06923401
C      -0.16807701     0.78280906     0.12180001
C       1.09519808     1.40427410     0.20142601
C       2.28112417     0.67530605     0.13538301
C       2.25662516    -0.72132105    -0.00603200
C       1.02682808    -1.33994610    -0.10466001
H      -6.02553543     1.13604008     0.13385501
H      -3.90447828     2.38992117     0.40494703
H      -3.79876727    -2.46955518    -0.49942104
H      -5.96580942    -1.30440709    -0.31944102
O      -1.32145610    -2.62336619    -0.47869303
O      -1.52013111     2.70048619     0.52993204
C       4.77360234     0.59984805    -0.15191001
C       4.74400234    -0.71756805    -0.29229102
H       5.70571039     1.13627808    -0.29358702
H       5.64936142    -1.25844509    -0.54500804
C       3.58261426     1.41926110     0.20862402
H       3.53435526     2.30262817    -0.43320303
H       3.70861927     1.82917613     1.21930909
C       3.51486725    -1.53464111    -0.08593501
H       3.63542726    -2.11998915     0.83438606
H       3.41101025    -2.28019716    -0.88040906
```

O	0.92992107	-2.69222320	-0.29302102
O	1.22431009	2.74463220	0.38098403
C	0.98976207	-3.48669225	0.89519607
H	0.32225402	-3.08321822	1.65584312
H	0.68374705	-4.48892732	0.61037504
H	2.01432515	-3.50223225	1.26879109
C	0.98808807	3.53220526	-0.78084805
H	-0.04237700	3.42876125	-1.11955508
H	1.17264508	4.56583533	-0.49544304
H	1.67738912	3.24701923	-1.58096311

*

serial number	Q4+H Minimized Geometry at Ground State		
level of opt &freq	PBE0, may-cc-pVTZ, DFT-D3(BJ), IEFPCM(acetonitrile)		
electronic energy		-1072.4133220 a.u.	
Temperature		298.150 K	
Thermal correction to U	907.146 kJ/mol	216.813 kcal/mol	0.345514 a.u.
Thermal correction to H	909.625 kJ/mol	217.406 kcal/mol	0.346458 a.u.
Thermal correction to G	721.848 kJ/mol	172.526 kcal/mol	0.274937 a.u.
Sum of electronic energy and thermal correction to G			
-1072.1383846 a.u.			

* xyz 0 2

C	5.04054629	-0.65317871	0.06805374
C	3.85299588	-1.30191456	0.32998830
C	2.63184654	-0.64070653	0.20263062
C	2.60126157	0.71624177	-0.18010505
C	3.82725658	1.36191786	-0.44463295
C	5.02016787	0.68897198	-0.32382556
C	1.39484183	-1.37744189	0.46715915
C	1.35142551	1.39122305	-0.25393937
C	0.11798267	0.70599960	-0.07479054
C	0.13825867	-0.71458011	0.11466178
C	-1.07506923	-1.41872841	0.07099938
C	-2.30428343	-0.75749827	0.00650331
C	-2.32970514	0.63506119	-0.04740634
C	-1.14049657	1.35254340	-0.09821600
H	5.98294778	-1.17796615	0.15873982
H	3.83783591	-2.34110867	0.63137979
H	3.86940545	2.39796535	-0.76258553
H	5.94758270	1.20519093	-0.53776457
O	1.43783498	-2.49040547	0.99920895
C	-4.81039762	-0.78337490	-0.09789904
C	-4.83912164	0.54139174	-0.13629018
H	-5.73955095	-1.34318563	-0.12311219
H	-5.79141953	1.05842131	-0.19264010
C	-3.55624931	-1.58110979	-0.01829598
H	-3.50597883	-2.28493780	-0.85726151
H	-3.58396045	-2.22881541	0.86587738
C	-3.62156235	1.39792587	-0.10795272
H	-3.67913163	2.08701235	0.74251790
H	-3.60709227	2.05725722	-0.98251701
O	-1.25281500	2.70811735	-0.20793254
O	-1.16435431	-2.76639745	0.09070702

C	-1.08231165	3.41140023	1.01506841
H	-0.08039196	3.26025986	1.42106903
H	-1.22459830	4.46699279	0.79175429
H	-1.82474909	3.09228033	1.75237694
C	-0.38090233	-3.53044452	-0.81655105
H	0.39867173	-4.06613704	-0.27953749
H	-1.05645309	-4.23243369	-1.30651348
H	0.08117851	-2.88829770	-1.56835405
O	1.32160047	2.70223835	-0.53589836
H	2.21867002	3.04688562	-0.57306922

*

serial number	Q4-H Minimized Geometry at Ground State		
level of opt &freq	PBE0, may-cc-pVTZ, DFT-D3(BJ), IEFPCM(acetonitrile)		
electronic energy		-1071.2023900 a.u.	
Temperature		298.150 K	
Thermal correction to U	843.609 kJ/mol	201.627 kcal/mol	0.321313 a.u.
Thermal correction to H	846.088 kJ/mol	202.220 kcal/mol	0.322258 a.u.
Thermal correction to G	662.346 kJ/mol	158.305 kcal/mol	0.252274 a.u.
Sum of electronic energy and thermal correction to G			
-1070.9501156 a.u.			

* xyz 0 2

C	5.01538071	-0.62821150	-0.15434187
C	3.84685987	-1.27992044	0.19787013
C	2.63795216	-0.59180738	0.18679578
C	2.60798168	0.75835171	-0.15156856
C	3.78940126	1.41426343	-0.48271038
C	4.98640821	0.72085494	-0.49615835
C	1.39206688	-1.30020447	0.54543374
C	1.34007751	1.52409493	-0.10021421
C	0.07508174	0.75046732	-0.00020384
C	0.12201334	-0.66445578	0.16589067
C	-1.06835298	-1.40446598	0.09475601
C	-2.30337346	-0.76656278	-0.01031230
C	-2.36273016	0.63137461	-0.10148451
C	-1.15807958	1.38143453	-0.10974713
H	5.95395204	-1.16818569	-0.16259652
H	3.85078631	-2.32597634	0.47450336
H	3.75094071	2.46770837	-0.72611601
H	5.90270889	1.22970680	-0.76798472
O	1.37373504	2.74046520	-0.16292476
O	1.44305289	-2.35951271	1.15466675
C	-4.80568527	-0.81306085	-0.16897651
C	-4.80897671	0.54504360	-0.25258002
H	-5.73699757	-1.36547935	-0.19347257
H	-5.74968888	1.07459147	-0.34656401
C	-3.55069709	-1.59423197	-0.04879890
H	-3.47932683	-2.32256964	-0.86869338
H	-3.59369952	-2.23366808	0.84388511
C	-3.61675510	1.28339614	-0.22871901
H	-3.63704787	2.35863967	-0.32525730
O	-1.28626550	2.71970584	-0.28567427
O	-1.13590370	-2.75117107	0.12289640

C	-1.26872423	3.48487553	0.91485015
H	-0.32361333	3.35782335	1.44324882
H	-1.38177493	4.52579561	0.61950268
H	-2.10165351	3.19568894	1.56190010
C	-0.27262758	-3.52143657	-0.70414265
H	0.49534974	-4.00390291	-0.10325319
H	-0.89401105	-4.27034034	-1.19456394
H	0.20379848	-2.89452401	-1.46008072

*